Experimental and Ab-initio Studies of Exotic Superconductors

Synopsis for Ph.D. in Physics

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1. Introduction

Superconductivity is one of the most fascinating and challenging fields in Condensed Matter Physics [1]. This phenomenon was first discovered by Kamerlingh Onnes in mercury (Hg) at ~4.2K, in 1911 [2], while studying its resistivity at low temperatures. It is a phenomenon by virtue of which below certain temperature called *critical temperature* a material can *conduct electric current without resistance*, i.e. without any loss of energy. Apart from perfect conductivity, *Meissner effect* is another fundamental property associated with a superconducting state, by virtue of which a superconductor expels out magnetic flux from its interior and can lead to its levitation in a magnetic field. Another novel property associated with a superconductor is quantization of magnetic flux i.e. magnetic flux entrapped in superconductor due to circulating current loops (vortices) is an integral multiple of unit $h/2e$ (where h is Plank's constant) called *flux quanta*. However, if applied magnetic field exceeds a certain limit called *critical magnetic field*, the material ceases to be a superconductor.

Since the discovery of this mysterious phenomenon, and the variety of materials which exhibit superconductivity [3][4][5]; it has been a challenging task to understand its mechanism. Even after hundred years of its discovery, not only the mechanism behind superconductivity for many materials is a mystery, but also the dream to realize this phenomenon at room temperature is one of the biggest challenges, which has led to an intense activity in this field involving basic researchers and technologists [6] working all around the world. Among the key requirements for superconductor applications are higher values of critical temperature and critical magnetic field up to which superconducting material can superconduct.

Ideally speaking a superconducting material makes generation of higher and higher magnetic fields possible without consumption of energy, and can make large distance power transmission lossless. Magnetic levitation (MAGLEV) via Meissner effect has led to an interesting application of superconductivity to significantly enhance the speed of long distance transport system through levitating trains. Other fascinating applications of superconductors include fault current limiters (FCLs), nuclear magnetic resonance (NMR) imaging (which requires high as well as extremely stable magnetic fields) and superconducting quantum interface device (SQUID) magnetometers that uses phenomenon of flux quantization and are capable of detecting very weak magnetic fields of the order of 10^{-14}T.

Till date superconductivity phenomenon has been observed at temperatures up to 165K. There has been extensive research worldwide during past one century to increase the critical temperature (T_c) from 4.2K for mercury to around 135K for high T_c cuprate ($HgBa_2Ca_2Cu_3O_x$), a superconductor [7], which shows superconductivity up to ~165K under high pressure [8][9]. Higher is the value of critical temperature easier will be to construct and maintain the cryogenic systems required to enjoy the applications using novel features of superconducting state. Elemental superconductors and most of their alloys exhibit superconductivity below 30K and are generally called *low temperature superconductors* (LTSCs). However, as mentioned above there are materials with complex structures that exhibit superconductivity up to as high as 165K which is the record value of T_c measured worldwide till date [10]. They are called *high temperature superconductors* (HTSCs). Superconductivity near room temperature [6] is a dream of superconducting researchers, which is yet to be realized.

Along with challenges in applied aspects of superconductivity, theoretically it is very difficult to explain its mechanism from microscopic considerations. Bardeen, Cooper and Schrieffer [3] (BCS theory) put forward the first microscopic theory to describe superconductivity at low temperatures, in terms of binding of electrons via an attractive interaction caused by phonons leading to the formation of *Cooper pairs* resulting in *Bose-Einstein condensation* of electron pairs. This leads to famous separation of superconducting ground state from normal state by an *energy gap* at Fermi level. This landmark theory has been successful in explaining many properties related to superconducting state. The materials that can be explained within BCS theory are termed as *conventional superconductors*. However, with time, there have been many surprising discoveries by experimentalists [4][5][7][11][12][13][14][15][16] which have led to a wide range of superconducting materials that

cannot be understood within BCS theory. These superconductors are termed as *unconventional or exotic superconductors.* The various classes of exotic superconductors are *heavy fermions*, *organic superconductors*, high T_c *cuprates* with the latest addition of *iron pnictides* and *iron chalcogenides*. The concept of Cooper pairs in superconductors has remained intact till date and most modern theories believe Cooper pairs to be a fundamental entity for precipitating superconductivity [17]. The mysterious part is the knowledge of mechanism behind Cooper pair formation [10][18]. Many of modern theories believe that the pairing of electrons in unconventional superconductors is mediated by dynamical magnetic interactions [19][20][21][22][23] and there are also many experimental evidences for that [24][25][26][27]. However, there is no detailed quantitative basic formalism that is able to account for and predict higher values of superconducting transition temperatures. In nutshell the phenomenon of superconductivity offers most attractive and challenging opportunities to the scientific community to unravel the mechanism behind the phenomenon.

2. Review of Literature

2.1 The Discovery: Work by Kamerlingh Onnes

One of the major causes believed to be leading to resistance of metals is associated with scattering of the conduction electrons by positive ions in the lattice. At higher temperatures, the vibrations of ions about their mean position within the lattice is supposed to lead to scattering of the conduction electrons and hence resistance. So, as the temperature is lowered, the amplitude of these ionic vibrations starts decreasing, resulting in smaller scattering cross section and hence lowering of resistance. Lord Kelvin [28] had also suggested that at very low temperatures, the conduction electrons would reattach themselves to the atoms and as a consequence would no longer be able to move freely, resulting in the electrical resistance passing through a minimum before rising rapidly. This idea motivated Kamerlingh Onnes to study the resistance of pure metals at lower temperatures [28]. In his pioneering experiments to obtain lowest temperatures, Onnes was able to obtain temperature as low as ~1 K. In contrast to gold and platinum studied, he found that for mercury (Hg) the resistance shows sharp drop below 4.2K and approaches zero within measurable limits, Figure 1 [2]. Similar behaviour was observed in both lead and tin at temperatures of 7.2 and 3.7K respectively. To make sure that electrical resistance was indeed zero, Onnes designed experiments that consisted of inducing a current into a superconducting loop and observing any decay in its magnitude, which was possible to notice as reduction in the associated magnetic field. To his surprise he found that no diminution in the current takes place even for years [29], phenomenon described as *persistence of current*. This established the fact that certain metals definitely lose their electrical resistivity completely below certain temperature called *critical temperature* (T_c) and the phenomenon was thus named as *Superconductivity*. This novel property of persistence of current was soon speculated as potential application for generation of high magnetic fields without any external source of voltage.

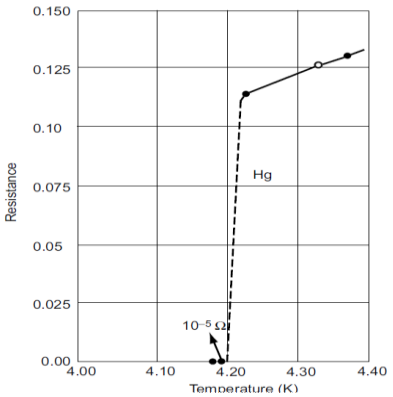

Figure 1: Resistance of mercury as function of temperature and observation of superconductivity

2.2 Effect of Magnetic fields

It was soon realized that passage of a large current produces a magnetic field which destroys superconductivity. There is a limit to the amount of current density that can be carried by a superconductor. This is known as the *critical current density* (J_c). In addition, application of a strong enough magnetic field also destroys superconductivity. This *critical magnetic field* (H_c), required to make the superconductor normal, is different for each superconducting material (Figure 2). Therefore, for any potential

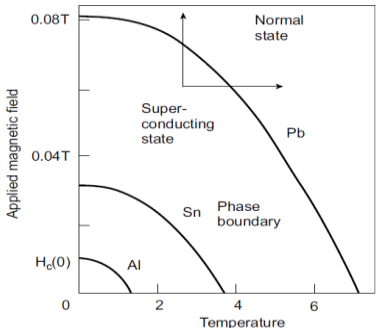

Figure 2: Critical magnetic field of different elements as function of temperature

application the superconductor should have higher values of these two *critical parameters*. In 1933, Walther Meissner and Robert Ochsenfeld discovered another fundamental property associated with superconducting state, namely perfect diamagnetism [30]. They found that any superconducting material when cooled below its critical temperature expels out all the magnetic field from its interior. This phenomenon is known as *Meissner effect*. The materials that strictly exclude all the magnetic flux, when in superconducting state, are called *type I superconductors*. There are some superconductors which do not expel external field completely and there is a mixed state in which both normal and superconducting regions coexist. These types of superconductors are known as *type II superconductors*. In this mixed state, a zero electrical resistance path through the superconducting regions still exists so that zero resistance is maintained. Type II superconductors can have substantially higher critical temperatures and magnetic fields than type I superconductor. This makes them potential candidates for applications in different areas.

2.3 Early attempts to understand Superconductivity

Among the earliest attempts to understand mechanism of superconductivity was proposed by C.J. Groter and H.B.G. Casimir [31] in the form of *two-fluid model*, which says that electron gas in superconductor has two components, one consists of *superelectrons* which are completely ordered and hence have zero entropy and carry the supercurrents, while the other component contains all the entropy of disorder and behaves like a normal electron gas. Below the superconducting transition temperature, ordinary electrons condense into pairs of electrons called superelectrons, which consist of electrons with opposite spins and equal and opposite momenta so that the net momentum and the net spin of the pair is zero. As the temperature lowers below T_c, the number of free electrons entering into the pair formation increases.

Another attempt to understand superconductivity was made by Fritz London and Heinz London [32] phenomenologically, who modified the classical Maxwell equations of electrodynamics by incorporating persistent currents leading to famous London phenomenological equations for superconducting state. The equations relate electric (E) and magnetic (B) fields inside a superconductor to the current density J as given below:

$$E = \mu_0 \lambda_L^2 \frac{dJ}{dt} \qquad \text{(1a)}$$

$$B = -\mu_0 \lambda_L^2 \nabla \times J \qquad \text{(1b)}$$

where λ_L is called London *penetration depth* and is given by $\lambda_L = \left(\frac{m}{\mu_0 n_S e^2}\right)^{\frac{1}{2}}$, m and e being electronic mass and charge respectively. With the help of these equations, they were able to predict that although magnetic flux is excluded from the interior of a superconductor, still there is a shallow surface region having a characteristic distance known as the penetration depth λ, in which there is some penetration of flux. Fritz London later suggested that superconductivity is a quantum mechanical state observable on a macroscopic scale [33].

The existence of magnetic fields in superconductors was found to be in the form of "*vortices*" by L. V. Shubnikov and co-workers [34]. They discovered the existence of two critical magnetic fields for type-II superconductors, the *lower critical field* H_{c1} and *upper critical field* H_{c2}. Below H_{c1} whole of the magnetic field is expelled out of the material and it becomes perfectly diamagnetic with χ=-1. For higher values of magnetic field, flux starts penetrating the sample though maintaining zero resistance state. The moment magnetic field exceeds H_{c2} the sample looses superconductivity and becomes a normal metal. The state of sample between H_{c1} and H_{c2} is known as the *mixed state* or *Shubnikov's phase*. V. Ginzburg and L. Landau [35] extended the London brother's phenomenological theory by using Landau's theory of second order phase transitions, by introducing the idea of an *order parameter*. Order parameter is a complex wave function of the superconducting electrons which distinguishes the superconducting phase from the normal phase. The Ginzburg-Landau theory provided new insights into the dependence of the critical field and current on temperature and thickness in thin films. They introduced the concept of a *coherence length,* which gives a measure of the distance between electrons in Cooper pair in zero magnetic fields. In 1957, Alexei Abrikosov [36] was able to use the Ginzburg-Landau theory as the starting point for his own classic work, which predicted type II superconductivity and showed that in the mixed state the

magnetic flux penetrates in a regular array of quantum vortices, later leading to an award of Nobel prize for him in 2003 [36].

2.4 BCS Theory: The microscopic description of superconductivity

The first microscopic theory of superconductivity, known in literature as *BCS theory* was proposed in 1957 by John Bardeen, Leon Cooper and J. Robert Schrieffer [3]. The key motivation behind this theory was experimental observation of *isotope effect* [37][38] in which it is observed that critical temperature T_c is inversely proportional to square root of the isotopic mass *M* of the comprising atoms of the material. This led Cooper to think of importance of lattice vibrations (*phonons*), as underlying mechanism to overcome coulomb repulsion among the electrons and binding them to form *Cooper pairs*. BCS theory has been successful in explaining superconductivity in many materials now known as *conventional superconductors*. As per BCS theory the superconducting transition temperature for phonon mediated superconductor is given by:

$$T_c = 1.14 \frac{\hbar \omega_D}{k_B} exp\left(\frac{-1}{N(0)V}\right) \qquad (2)$$

where, ω_D is Debye frequency, k_B is Boltzmann constant, *N(0)* is electronic density of states at Fermi level, *V* is pairing potential arising due to electron-phonon interaction.

However, one disappointing prediction of BCS theory was that there is an upper limit for T_c, and that superconducting material can exhibit maximum T_c of ~30K [3][39]. Among the conventional superconductors, MgB_2 is the material with highest T_c (~39K) which can be explained within BCS strong coupling limits [40]. Despite the discovery of many superconductors having T_c higher than BCS limits and with phonon independent pairing mechanisms, BCS theory has been to the date, the most successful and undisputed microscopic theory of superconductivity. Some of the ground breaking successes of BCS theory were: concept of Cooper pairs, quantitative prediction of *superconducting energy gap* at Fermi Surface (FS) and its temperature variation, jump in *electronic specific heat* at T_c and its exponential decrease with temperature below T_c, correct prediction of *Meissner effect* and *isotope effect*, variation of *critical magnetic field* with temperature [3].

B. D. Josephson, a young theorist of that time, theoretically predicted [41] quantum-mechanical tunnelling of Cooper pairs through a thin insulating barrier (of the order of a few nanometers thickness) between two superconductors. This prediction by Josephson was confirmed within a year and the phenomenon is now known as the Josephson effect. This effect plays a crucial role in superconducting applications such as Superconducting Quantum Interface Devices (SQUID).

2.5 The Breakthrough: Advent of *Exotic Superconductors*

After the success of BCS theory, scientists who were working in the field of superconductivity could relax and enjoy it during 1960s and 1970s. But then new superconducting materials were discovered namely, *organic superconductors* (Bechgaard salt) [42] and heavy fermions (such as $CeCu_2Si_2$, $CeRhIn_5$, $CeIn_3$) [14][15]. The experimental measurements on these materials indicated that these compounds display an *unconventional* type of superconductivity not explainable within BCS theory. Then, in the year 1986 the scientific world was surprises with the results of Müller and Bednorz who discovered superconductivity with T_c of ~30K in *ceramic material* $La_{2-x}Ba_xCuO$ conventionally an insulator, having layers of copper oxide (cuprates) [4]. The event was marked as beginning of the discovery of High Temperature Superconductivity (HTSC), since no material exhibited such high value of T_c at that time. Soon superconductivity was discovered in $La_{2-x}Sr_xCuO_4$ system with T_c of ~39K in the same year [43][44]. T_c sharply increased to 90K for YBCO [11], 110K for BSCCO [12] and 127K for TBCCO [13] systems. Till date, the highest T_c superconductor (at ambient pressure) is $HgBa_2Ca_2Cu_3O_x$, at 135K [7], which further reaches 164K under high pressure [8][9]. All the cuprate superconductors have layered structure which consists of Cu-O planes responsible for hosting superconductivity. Interestingly, the discovery of cuprate superconductors has raised the superconducting transition temperature well above liquid nitrogen temperature.

Recently, Fe-based superconductors (FBS) with critical temperatures as high as 56K have also been discovered [5]. These are also referred to as high-temperature superconductors, though they are different from ceramic superconductors. These materials are broadly classified into four different classes depending upon the chemical formula of the parent compound. These are LaFeAsO (1111),

$BaFe_2As_2$ (122), LiFeAs (111) and FeSe (11). These materials have many similarities with cuprates. They are also layered materials like cuprates and as Cu-O layers are key elements for superconductivity in cuprates, layers of Fe-X (X=pnictogen or chalcogen) plays central role in superconductivity of FBS. Parent compounds for both cuprates and FBS materials have antiferromagnetic (AFM) ordering and doping by charge carriers (electrons or hole) suppresses the AFM ordering thereby creating conditions for formation of Cooper pairs. One major difference between cuprates and FBS is that parent compounds in case of cuprates are insulators, which is attributed to strong correlations of electrons in these materials. However, parent compounds for FBS are metals and do not exhibit strong correlations. Highest value of T_c for FBS reported till date is 56K for $Sm_{0.5}Sr_{0.5}FeAsF$ (1111). Most striking feature of these materials is that the electron pairing is not mediated by phonon and is still not very clearly understood [45]. In these materials, magnetic interactions are speculated to play crucial role for pair formation [17][21][22][23]. This is in contrast to conventional superconductors where magnetic impurities if present results in degradation or even complete loss in superconductivity. Because of these facts these superconductors are also termed as *unconventional* or *exotic superconductors* [46].

2.6 Understanding Exotic Superconductivity

2.6.1 Cuprates

The mechanism of superconductivity in exotic superconductors is still not very well understood with many grey areas [18]. The general BCS concept of a macroscopic quantum state of Cooper pairs remains the common basis in almost all theories proposed for these superconductors. However, there is no consensus about the mechanism involved in pairing of electrons. It is expected that the lack of an isotope effect in HTSCs of highest T_c should favour a non-phonon pairing mechanism as, for instance, *d-wave pairing*, whereas its presence in several HTSCs with lower T_c suggests a phonon-mediated *s-wave pairing*.

In an effort to explain the superconductivity in heavy fermions, K. Miyake, S. Schmitt Rink and C. M. Varma [19] considered the mechanism of superconductivity based on the exchange of antiferromagnetic spin fluctuations. By observing the layered structure of cuprate superconductors, Krezin and Wolf proposed a model of high-T_c superconductivity based on the existence of two gaps one superconducting and another induced [47]. Later, Gorkov and Sokol proposed the presence of two component features, itinerant and more localized electrons in cuprates [48]. A. S. Davydov [49] has suggested that unconventional superconductivity in materials such as organic superconductors, occurs due to the formation of *bisolitons*. Davydov extended this theory to high-T_c superconductivity, based on the concept of a moderately strong electron-phonon coupling in cuprates due to which perturbation theory becomes invalid [50][51].

P. W. Anderson proposed that in cuprates, the electron pairing mechanism and the mechanism for the establishment of long range phase coherence are different [20]. Based upon this idea of Anderson, some theorists proposed that, independently of the origin of pairing mechanism, spin fluctuations mediate the long-range phase coherence in cuprates. This suggestion is being supported by many experimental observations [52][53][54].

The *pseudogap* above T_c [55] was observed using nuclear magnetic resonance (NMR) measurements [56]. The pseudogap is a partial energy gap caused by a depletion of the density of states at Fermi level and exists below certain temperature termed as T*. The pseudogap corresponds to a charge gap on charge stripes observed in copper oxide layers so that in order to pull electron or hole from such charge stripes charge gap must be overcome. Cooper pair formation occurs below temperature (T_{pair}) which can be observed even above the critical temperature and contributes further to pseudogap. Alexandrov and Mott pointed out that, in cuprates, the internal wave function of a Cooper pair and the order parameter of the Bose-Einstein condensate may have different symmetries [57] and must be distinguished from each other. Later, Emery and Kivelson emphasized that superconductivity requires not only pairing but also long-range phase coherence of superconducting wave functions [58]. They demonstrated that, in cuprates, the pairing may occur above T_c without the phase coherence.

J. M. Tranquada and co-workers observed the presence of coupled, dynamical modulations of charges and spins in Nd-doped La-Sr-Cu-O (LSCO) system from neutron diffraction [59]. In LSCO, antiferromagnetic stripes of copper spins are separated by periodically spaced quasi-one dimensional domain walls in which the holes segregate. Based on these observations, Emery, Kivelson and Zachar presented a theoretical model of high-T_c superconductivity [60] based upon charge-spin separation in cuprates. Though it was found that the model is incorrect and there is no charge-spin separation in cuprates; however, it is the first model of high-T_c superconductivity based on the presence of charge stripes in planes. The analysis of tunneling and neutron scattering measurements in Bi-2212 and YBCO showed that, the phase coherence is established due to spin excitations [61][62] which causes the appearance of the magnetic resonance peak in inelastic neutron scattering spectra [63]. Tunneling measurements also provided evidence that the quasiparticle peaks in tunneling spectra obtained in Bi-2212 are caused by condensed soliton like excitations which form the Cooper pairs [64][65][66].

2.6.2 Fe based materials

The discovery of superconductivity in the iron based compounds was surprising because iron being ferromagnetic, had long been considered detrimental to superconductivity. Unlike cuprates all five *3d* orbitals of Fe are involved in electronic structure near Fermi level [67]. Although, the parent compound in FBS is also antiferromagnetic as in cuprates but they are metals in their normal state for former whereas are insulators for later. Investigation of electron-phonon coupling for LaNiPO, which is isostructural with 1111 compounds, showed [68] that the superconductivity in this material can be explained within electron-phonon interaction. The value of electron-phonon coupling constant for Fe based materials has been found within a range of 0.12-0.25 [69] which is too small to account for higher values of T_c observed. Several groups have argued that since the strong magneto-elastic coupling in these materials has not yet been considered within the theory for superconductivity via the electron-phonon mechanism, it is premature to conclude that the electron-phonon mechanism is not relevant to these materials [70][71][72]. The presence of isotope effect in some of these materials indicates that the magnetism and superconductivity are both somehow coupled to phonons [73] in these materials.

Moreover, theoretical calculations by Kuroki et. al. [74] shows that height of anion atoms above Fe layers could be acting as a switch between high-T_c nodeless and low-T_c nodal pairings for Fe based superconductors. Based on this idea Mizuguchi et. al. [75] using experimental data have found interesting relationship between superconductivity and height of anion atoms above Fe layers for different classes of Fe based superconductors. They found that for optimally doped compounds, the superconducting transition temperature T_c shows a peak for height value of 1.38Å, above and below which the value of T_c decreases sharply. Based on DFT calculations Kuchinskii et. al. [76] have found that variation of T_c as function of anion height is due to the corresponding change in the density of states at the Fermi level and can be explained semi-quantitatively using BCS theory. They also suggested possibility of non-phonon pairing in region of maximum T_c.

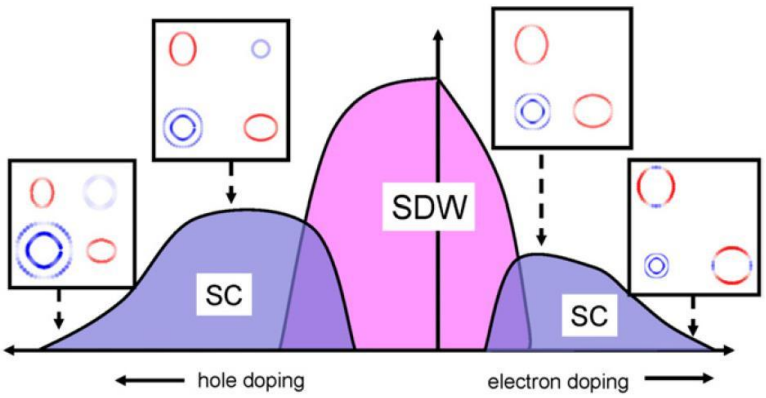

Figure 3: Typical phase diagrams for FBS. The circles in squares represent Fermi surfaces for various doping [77]. The Y-axis represents temperature scale (a.u.).

The typical phase diagram [77], Figure 3, of all these superconductors shows that antiferromagnetic ordering of parent compounds need to be suppressed for superconductivity to appear. This idea motivated many researchers to think of dynamic rather than static antiferromagnetism (or AF spin fluctuations) favouring high-temperature superconductivity [21]. This idea is supported by many experimental and theoretical findings. DFT based calculations on these materials shows that they have many bands crossing at Fermi level and disconnected cylindrical

Fermi surfaces [21][22][67][77]. For systems with multiple Fermi surfaces, the scattering of an electron pair from one FS to another is possible. Generalization of the BCS theory for the superconductors with two Fermi surfaces [78] has shown that it is possible to obtain superconductivity even when both the intra and inter FS pair scattering are repulsive provided that the inter FS pair scattering dominates [17]. Moreover, under this condition, the order parameter should have an opposite sign on the two Fermi surfaces. On the basis of these observations, Mazin et al. [21] have speculated that antiferromagnetic spin fluctuations can induce the $s_{\pm}$ pairing. Here, *s* refers to the fact that the order parameter is unchanged by the symmetry operations of the crystal, and ± refers to the sign change of the order parameter between the electron and hole like Fermi surfaces.

It is proposed by Korshunov et al. [79] and Maier el al. [80] that if pairing symmetry of order parameter is $s_{\pm}$ one expects a peak in neutron resonance scattering at ordering wave vector when system enters into superconducting state. This peak has been observed experimentally by Lumsden et. al. [81] thus supporting the idea of $s_{\pm}$ pairing. Another support to $s_{\pm}$ symmetry is provided by scanning tunneling spectroscopy experiments based upon scattering of quasiparticles by impurities. It is predicted [82][83] that if the superconducting order parameter has opposite signs on electron and hole Fermi surfaces, it will impact the elastic scattering of quasiparticles by impurities. Specially, the nonmagnetic impurities will scatter quasiparticles from hole to electron FS (and vice versa), but not from hole to hole or from electron to electron FS. If the impurities are magnetic, the reverse is true. This behaviour is recently observed in some measurements on Fe_{1+x}(Se,Te) [27] system giving further support to $s_{\pm}$ pairing.

The predictions of simplest $s_{\pm}$ pairing symmetry suggest nodeless superconducting gap. However, the order parameter can vary substantially around different Fermi Surfaces as suggested by various authors in [22][23][84]. In certain cases, this variation can also be such that nodes are produced in superconducting gap along certain directions [84][74]. A node in the superconducting gap is the location on the FS where the energy gap vanishes. Measurements of the superconducting gap in $Ba_{0.6}K_{0.4}Fe_2As_2$ by angle-resolved photoemission spectroscopy have revealed almost uniform gap on all observable Fermi Surfaces [85][86]. There is also experimental evidence for the existence of gap nodes in some FBS materials [87][88][89][90][91]. Recently some studies have provided a direct comparison between the results of the surface sensitive scanning tunneling spectroscopy measurements [27] and a bulk sensitive, angle-resolved specific heat measurement for Fe_{1+x}(Se,Te) [92]. Among these studies the tunneling spectra of Hanaguri et al. [27] indicate Fe_{1+x}(Se,Te) to be nodeless superconductor and the results of Zeng et al. [92] shows evidence for either nodes or minima of the energy gap. Chubukov et al. [93] and Vorontsov et al. [94] have argued that these results are consistent in case the nodeless gap exhibits angular variation. Thus, it seems that substantial evidence supports the notion that at least one FBS ($Ba_{0.6}K_{0.4}Fe_2As_2$) compound shows *s*± pairing. Though, it will not be wrong to say that antiferromagnetic spin fluctuations do play a crucial role for high T_c of both FBS and cuprates. More rigorous theoretical and experimental studies are needed to investigate detailed origin of pairing in these compounds.

3. Characterization techniques

Various characterization techniques play crucial role in understanding the properties of a material and underlying mechanisms. This characterization can be undertaken by many experimental techniques or through theoretical techniques such as ab-initio density functional calculations [95]. As an experimental part, synthesis of various superconducting samples is done by conventional solid state reaction route. Structural, electrical, magnetic and thermal properties of these samples then are studied employing different techniques. To get in depth understanding of microscopic properties, theoretical investigation is carried by using ab-initio density functional theory (DFT) based studies. In this study we shall use both techniques as described below.

3.1 Experimental Techniques

3.1.1 Sample synthesis by solid state reaction route

In solid state reaction route the oxide or carbonate powders of reactants are mixed in stoichiometric ratios and heated at various temperatures near crystallization temperatures till one obtains the required phase. All the samples in the present study will be synthesized via solid-state reaction route. In such reaction, the material transport occurs due to diffusion of atoms/ions through volume, surface and grain boundaries. Samples proposed for study are Bismuth based (BSCCO) cuprate superconductors, some interesting conventional superconductors such as MgB_2, $MgCNi_3$, Bi_3Ni and recently discovered Iron chalcogenides superconductors.

Three main terms referred to solid state reaction route are *Calcination, Sintering and Annealing.* **Calcination** is a thermal treatment process applied to ores and other solid materials in order to bring about a thermal decomposition, phase transition, or removal of a volatile fraction. **Sintering** on the other hand is a method for densification and increasing the average grain size of the material, by heating the material in a furnace below its melting point until its particles adhere to each other. Sintering is traditionally used for manufacturing *ceramic* objects. **Annealing** refers to the heat treatment wherein a material is altered, causing changes in its properties such as hardness, ductility, relieve internal stresses, refine the structure by making it homogeneous, and improves cold working properties. The samples can also be annealed in different gas environments to control oxygen content in stoichiometry.

3.1.2 Properties measurement

In this study the prepared samples will be measured for their structural, microctructural, electrical, magnetic and thermal properties. The results will be analysed by various techniques discussed below.

(a) Structural Studies

(i) X-Ray Diffraction (XRD)

XRD is one of the most important tools used for structural characterization of crystalline materials. The crystals are the materials with regular array of atoms or molecules in the space. When x-rays are incident on a crystalline material they gets scattered by the atoms into different directions. Due to periodic nature of atomic arrangement in the crystals, the intensity of scattered x-rays have maxima and minima in certain directions, depending upon whether they interfere in constructive or destructive manner. The condition for constructive interference is given by well known Bragg's law [96]:

$$2dsin\theta = n\lambda \qquad (3)$$

where *n* is an integer called order of diffraction, λ is the wavelength of x-rays used and θ is the angle between incident ray and scattering planes. Thus, when we shine x-rays on a crystalline material we find a pattern of high intensity peaks at certain angles according to Bragg's law. This pattern depends on the nature and periodicity of atomic arrangement in the crystalline material and thus helps in determining the structure.

The XRD pattern of a material is used to find unit cell parameters and atomic positions within a unit cell. For polycrystalline samples, crystallographic information about the different phases present, presence of impurities, average crystallite size and size distribution can be obtained from the analysis of the XRD pattern of a material.

(ii)Rietveld analysis

Rietveld refinement is a technique devised by Hugo Rietveld [97] for the characterization of crystalline materials. The neutron and x-ray diffraction of crystalline samples result in a pattern characterized by reflections (peaks in intensity) in certain directions. The height, width and position of these reflections can be used to investigate structural or even magnetic (in case of neutron diffraction) details of a material. Diffraction from single crystals give a set of well separated peaks from which the

structure can be obtained where as diffraction from powdered samples may result in overlapping of nearby peaks. This method creates a virtual separation of these overlapping peaks, thereby allowing an accurate determination of the structure even from diffraction pattern obtained using powdered samples. The Rietveld method uses a least squares approach to refine a theoretical line profile until it matches the measured profile. FullProf Suite [98] is a collection of softwares available which have been mainly developed for Rietveld analysis of neutron or x-ray diffraction data. In addition, magnetic profile refinement, multi phase analysis and profile matching can also be done using this suite.

(iii) Microstructural studies using Scanning Electron Microscopy (SEM)

An efficient way to obtain images of the surface of a specimen is to scan the surface with an electron beam. Surface information is obtained by scanning probe in which the trajectory of electron beam is directed across the region of particular interest on the surface. The SEM [99] is a type of electron microscope capable of producing high-resolution images (magnified by 10 to 500,000 times) of a sample surface to give details of even less than 1.0 *nm*. SEM images have a characteristic three-dimensional appearance and are useful for analysing the surface morphology, porosity and secondary phases of the sample.

(b) Electrical properties

(i)DC Transport or Resistivity versus Temperature (R-T) measurement

Four probe method is one of the standard and most widely used techniques, for the measurement of the resistivity of a material in Solid State Physics. This method becomes important when extremely small resistances are to be measured and where contact resistances become a crucial issue. In this method four silver paint contacts are made on the sample. Current is passed from a constant current source by the outer two contacts and the voltage is measured by a nano-voltmeter using the two central contacts. The four probe method isolates the current and voltage contacts which excludes the contact resistance from measured value. This method is illustrated in Figure 4.

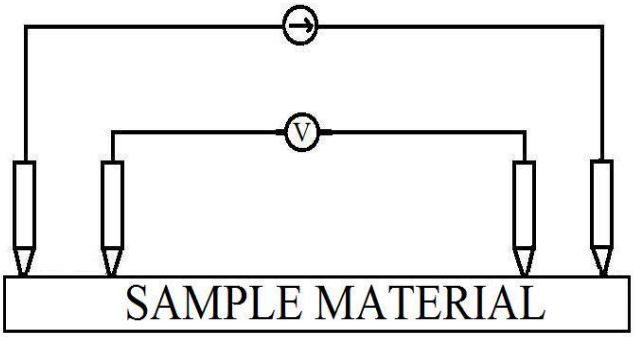

Figure 4: Schematic representation of four probe method

To study the superconducting transition, the resistance is measured at various temperatures below room temperature. The temperature is varied in a controlled manner using close cycle refrigerator (CCR) equipped with a temperature controller.

(ii) Thermoelectric power

The thermoelectric power of a material is the measure of voltage induced across it when a temperature gradient is set across its two ends. This is measured in micro-volts per Kelvin (μV/K). This is an important characterization that gives us information about majority charge carriers in the material. In addition, thermoelectric power becomes zero when material enters superconducting state as no voltage can exist across a zero resistance material. Thus we can also see superconducting transition by measuring thermoelectric power with temperature.

(c) Magnetic properties

The magnetic properties of the superconductors are interesting to investigate. While type I superconductors expel out the magnetic flux on superconducting transition, a type II superconductors

has much more interesting properties due to existence of vortices in the mixed state. The magnetic properties are measured by using different techniques like dc magnetization using vibrating sample magnetometer (VSM), ac susceptibility and magneto-resistance. All these will be carried out using Physical Property Measurement System (PPMS) of Quantum Design (QD).

(i) DC magnetization using Vibrating Sample Magnetometer (VSM)

When a sample is placed inside a magnetic field, it is magnetized depending upon its magnetic character. VSM is based on measuring the rate of change of magnetic flux due to the mechanical vibration of the magnetized sample, which produces an induced e.m.f. in a detection coil system. In PPMS the sample is placed in a uniform dc magnetic field produced using a superconducting magnet (placed in a liquid He Dewar), which is then made to oscillate sinusoidally with small fixed amplitude (~1.5mm). This produces an induced e.m.f. in the detection coil depending upon nature and magnitude of the magnetization produced in the sample. In present case the samples will be studied in temperature range of 4K to 300K and a magnetic field of 0 to 14T using Quantum Design PPMS.

(ii) AC susceptibility

The principle of measuring AC susceptibility involves subjecting a sample to a small alternating magnetic field. In the susceptometer two sensing coils are positioned symmetrically inside the primary coil and serve as the secondary coils in the measuring circuit. The two sensing coils are connected in opposition in order to cancel the voltages produced by ac fields itself or any other external unwanted sources. The sample is inserted in one of the secondary coils. The surrounded sensing coils pick up the flux variation due to the sample and the resulting voltage induced in them is detected. This voltage is proportional to the time derivative of the sample's magnetization. Thereby using the concept of mutual inductance, AC magnetic susceptibility is obtained. Using Quantum Design PPMS, the AC susceptibility will be measured within temperature range of 4K to 300K and a DC magnetic field up to 14T in present study.

(iii) Magneto-resistance

Magneto-resistance is measured using four probe technique in the presence of applied magnetic field. Four silver contacts are made with thin copper wires on the sample. Current is passed from a constant current source by the outer two wires and the voltage is measured by a nano-voltmeter using the two central wires. Magnetic field can be varied from 0 to ± 14 T in the temperature ranging from 4K to room temperature. Magneto-resistance studies in superconductors are used to investigate important details of vortex dynamics for various superconducting samples in present study.

3.2 Theoretical Techniques

All the matter around us is made up of atoms and molecules which further consist of electrons and nuclei. Quantum mechanics has proven to be best formulation to describe interacting system of electrons and nuclei. Schrodinger equation is the fundamental quantum mechanical equation that describes a system of electrons and nuclei in terms of *wave function* ψ, which is a fundamental entity in quantum mechanics. The Schrodinger equation for an *N*-electron system is as given below:

$$\left[-\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i,I}\frac{Z_I e^2}{|r_i - R_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|} - \frac{\hbar^2}{2M_I}\sum_I \nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|R_I - R_J|}\right]\psi = E\psi \qquad (4)$$

The different terms under summation in brackets on left hand side are kinetic energy of electrons, potential energy of electrons with different nuclei, Coulomb potential energy between various electrons, kinetic energy of various nuclei and electrostatic potential energy of different nuclei respectively. The most challenging task is to obtain solution of this Schrodinger's equation for many electron systems and this requires many judicious approximations without significantly affecting involved physics in the system. One of the approximations is based upon the idea that mass of the electrons is much smaller that of nucleus and thus electrons move much faster than nucleus. Thus for

a given set of positions of nuclei, electrons adjust almost *immediately* to these before nuclei move. This is known as *Born-Oppenheimer approximation*. With inclusion of this approximation term corresponding to kinetic energy of nuclei that originates from the electronic pert of the wave function can be neglected. This approximation is very important starting point for perturbation theory in electron-phonon interaction which is a basis for the understanding of many properties like electrical transport in metals, polaron formation in insulators, metal-insulator transitions and BCS theory of superconductivity. Another approximation called *independent electron approximation* which assumes electrons to be non-interacting with each other; however they obey Pauli's exclusion principle. This approximation is employed in Hartree-Fock method and allows us to express total Hamiltonian for *N*-electron system (H_i) as summation of single electron Hamiltonian (h_i) i.e. $H_i = \sum_i h_i$ and total wave function as Slater determinant of single electron wave functions. Figure 5 describe various terms and concepts involved when we come across various theoretical and computational methods to solve Schrodinger equation. Our interest is in solving Schrodinger's equation by means of ab-initio Density Functional Theory (DFT) as described below.

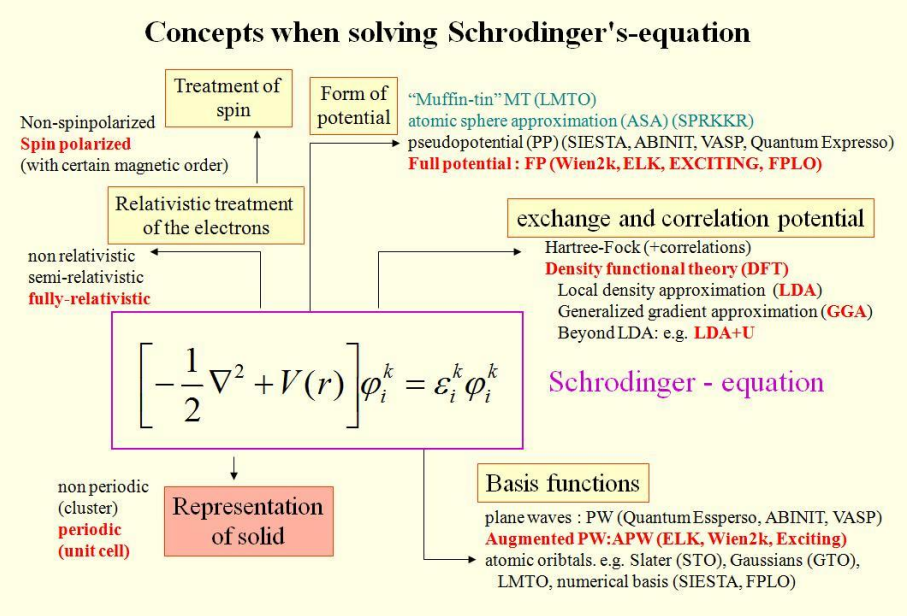

Figure 5: Concepts involved in solving Schrodinger equation [121]

3.2.1 *Ab initio* study using Density Functional Theory (DFT)

The term *ab initio* originates from Latin word meaning *from the* beginning. A method is said to be *ab initio* or from first principles if it relies on basic and established laws of nature without additional assumptions or special models based upon particular material. Density functional theory (DFT) is an extremely successful ab-initio approach to compute properties of matter at microscopic scales. DFT is a quantum mechanical modelling method used in physics to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases (bulk, surfaces, chains). The fundamental concept behind density functional theory is that charge density (3-Dimensional) can correctly describe the ground state of *N*-particle instead of explicit usage of wave function (3*N*-Dimensional) [100].

The fundamental pillars of density functional theory are two physical theorems proved by Kohn and Hohenberg [101]. The first Hohenberg Kohn (HK) theorem states that: *The ground-state energy from Schrodinger's equation is a unique functional of the electron density*. This theorem provides one to one mapping between ground state wave function and ground state charge density. We may also state first HK theorem as: *The ground state charge density can uniquely describe all the ground state properties of system.* Thus by using charge density instead of wave functions a 3*N* dimensional problem reduces to a 3 dimensional problem. The second HK theorem states that: *The electron density*

that minimizes the energy of the overall functional is the true electron density corresponding to the full solution of the Schrodinger equation. If the *true* functional form of energy in terms of density get known, then one could vary the electron density until the energy from the functional is minimized, giving us required ground state density. This is essentially a variational principle and is used in practice with approximate forms of the functional designed by quantum chemists/physicists to study different types of systems [95].

The simplest possible functional is choosing constant electron density all over the space. The total charge density can be written in terms of single particle wave functions as:

$$n(\mathbf{r}) = 2\sum_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) \qquad (5)$$

where the factor of 2 appears because of two spin orientations of electrons. To obtain the single particle wave functions Kohn Sham (KS) [102] equations are used which correspond to Schrodinger equation for a fictitious system with non-interacting electrons that generate same density as that of a given system of interacting electrons would. The KS equations are defined by a local effective external potential (called Kohn Sham potential) in which the non-interacting particles move. The Kohn–Sham equations have the form

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + V_H(\mathbf{r}) + V_{XC}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r}) \qquad (6)$$

On the left-hand side of the Kohn-Sham equations there are three potentials, V, V_H, and V_{XC}. The first potential defines the interaction of an electron with different atomic nuclei present. The second is called the Hartree potential. This potential describes the Coulomb repulsion between the electron being considered in one of the Kohn-Sham equations and the total charge density defined by all electrons in the problem. The Hartree potential includes a so called self-interaction contribution because the electron we are describing in the Kohn-Sham equation is also part of the total electron density, so part of V_H involves a Coulomb interaction between the electron and itself. The self interaction is unphysical, and the correction for it is one of several effects that are lumped together into the final potential in the KS equations, V_{XC}, which defines exchange and correlation contributions to the single electron equations.

To solve KS equation we need Hartree potential which depends upon the charge density of the system and to know the charge density we need the single particle wave functions, which can be obtained only after solving KS equations. Thus the problem reduces to solving a set of self consistent equations. They are solved in an iterative way by starting with a trial set of single particle wave functions from which Hartree potential is obtained. The solution obtained in this way is called self consistent solution. The algorithm used to solve it is as given in figure 6:

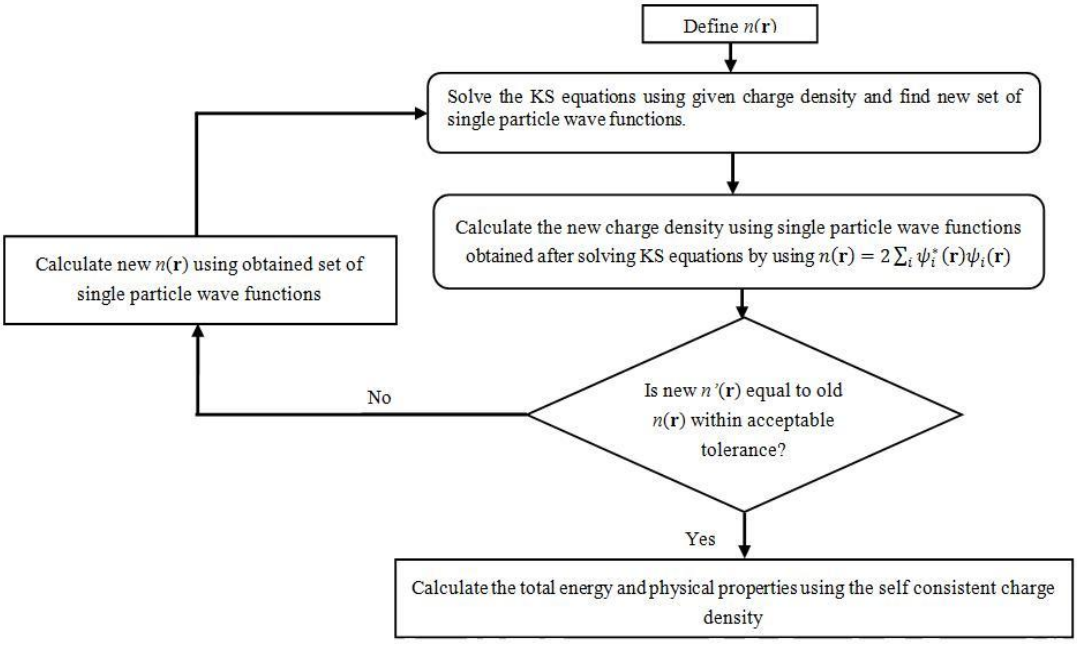
Define $n(\mathbf{r})$
Solve the KS equations using given charge density and find new set of single particle wave functions.
Calculate the new charge density using single particle wave functions obtained after solving KS equations by using $n(\mathbf{r}) = 2\sum_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r})$
Is new $n'(\mathbf{r})$ equal to old $n(\mathbf{r})$ within acceptable tolerance?
No
Calculate new $n(\mathbf{r})$ using obtained set of single particle wave functions
Yes
Calculate the total energy and physical properties using the self consistent charge density

Figure 6: Algorithm to solve Kohn Sham equations in DFT Codes

One of important potential term in KS equations is V_{XC} which is used to describe exchange and correlation effects. Unfortunately, exact form of the exchange correlation functional whose existence is guaranteed by the Hohenberg-Kohn theorem is not known. But, there is one case of uniform electron gas where this functional can be derived exactly as the electron density is constant at all points in space. Therefore, the exchange-correlation potential at each position is set to be the known exchange-correlation potential from the uniform electron gas at the electron density observed at that position. This approximation uses only the local density to define the approximate exchange correlation functional, so it is called the *local density approximation* (LDA) [103]. Although, LDA gives a way to completely define the Kohn-Sham equations, but these equations do not exactly solve the true Schrodinger equation because the true exchange correlation functional are not being used. Apart from LDA, many other functionals tailored to explain properties of particular systems have been tried for DFT calculations. After LDA, the best known class of functional that has been defined is *generalized gradient correction* (GGA). GGA uses information about the local electron density and also the local gradient in the electron density [104]. Though GGA includes more physical information than LDA, it is not necessary that it must be more accurate. There are a large number of distinct GGA functionals depending on the ways in which information from the gradient of the electron density can be included in a GGA functional.

As has been discussed already that superconductivity is most mysterious state of matter till date and so is the exact theoretical formulation of this state. However, study of normal state properties of superconducting materials provides us many important clues to demystify the phenomenon of superconductivity. Density functional theory has been a very useful tool to study normal state properties of superconducting materials and provide many important theoretical clues about microscopic nature of the system. For example when the parent compounds of cuprate superconductors are studied using band theory, they were found to be metals. However, experimentally they are found to be insulators. This led to very important concept of strongly correlated electrons in these systems [105]. Moreover, density functional theory has been successful in predicting observed magnetic ground state of the parent compounds [106][107][108]. Whether magnetism is important in the given system or not can be studied by using density functional theory [109]. The study of electron-phonon correlations in superconductor is another interesting aspect which can be probed using density functional theory within BCS formalism [67][40][110][111][112].

3.1.3 Different Codes to perform DFT calculations

Today many open source and proprietary computer codes are available which provide a way to calculate various properties of materials using density functional theory. These codes differ in terms of their implementations used to solve KS equations. Depending on how atomic electrons are treated they are termed as full potential (FP-Wien2k [113] and ELK [114]), pseudopotential (SIESTA [115], CASTEP [116]), atomic sphere approximation (ASA-SPRKKR [117]) or Muffin tin (LMTO [118]) based. They are also classified depending upon what basis set is used to expand wave function. Various methods use plane wave (PW) (Quantum Essperso, ABINIT, VASP, CASTEP), augmented plane wave (APW) (ELK, Wien2k, EXCITING) or localised atomic orbitals as basis sets (SIESTA, FPLO) [119]. In the following is given a brief description of some of available codes which are proposed to be used to calculate the electronic properties of different materials using DFT.

(a) Wien2k code

Wien2k [113] is the code that can be used to study ground state properties of materials based upon density functional theory. This code uses all electron, full potential linearized augmented plane wave (FP-LAPW) method to calculate different electronic properties of a material. LAPW method is among most accurate methods to determine electronic properties of crystalline materials. Different formulations for exchange and correlation effects, like LDA and GGA by various authors, are available [120].

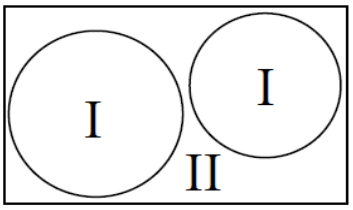

Figure 7: Division of crystal unit cell into two regions in LAPW [121].

In LAPW method the whole space in unit cell is divided into two regions: one containing non-overlapping atomic spheres centred at atomic positions and another consists of region outside spheres called interstitial region. Different basis sets are used in these two regions. In region I inside atomic spheres, the linear combination of radial wave function and spherical harmonics is used that represents solution of Schrödinger equation for that atomic species. In the second region called interstitial region, (Figure 7) a plane wave expansion is used as basis set. The solution of KS equations is expanded in linear combination of this combined basis set of LAPW's. These equations are then solved self consistently to obtain the ground state solution to the problem. From where various properties such as electronic density of states, band structure, Fermi surfaces etc. can be calculated. Different magnetic or disordered states can be modelled by using supercell approach.

(b) ELK code

This code is also based upon FP-LAPW method and is an open source program [114]. This code can be used to calculate many properties apart from ground state electronic structure particularly targeted to look at properties relevant for superconducting systems. This code allows electron-phonon interactions and calculations of phonon density of states, phonon dispersion plots, Eliashberg function, electron-phonon coupling constant and superconducting transition temperature within McMillan Allen Dynes approach. Optical properties using random phase approximation (RPA), time dependent density functional theory (TDDFT) and Bethe Salpeter Equations (BSE) are also possible in this code. We can perform fixed spin moment calculations for magnetism by fixing total moment on unit cell or within atomic spheres. Moreover, different calculations can be performed using various features of code in parallel to each other. For example electron-phonon spectra can be calculated by considering LDA+U or spin-orbit coupling. This makes ELK code very efficient and flexible to model different states of material and compute its properties.

(c) SIESTA code

SIESTA [115][122] (Spanish Initiative for Electronic Simulations on Thousands of Atoms) is an ab-initio method based upon density functional theory to perform electronic structure and molecular dynamics simulations of molecules and solids. It uses norm-conserving pseudopotentials in their fully nonlocal (Kleinman-Bylander) form. Atomic orbitals are used as a basis set, allowing inclusion of unlimited multiple-zeta and angular momenta, polarization and off-site orbitals. This is an efficient code to perform DFT calculations on systems containing large number of atoms. One of the most interesting features of SIESTA is availability of TransSiesta in it. Using TransSiesta, one can calculate electronic transport properties such as, zero bias conductances and the I-V characteristics, of a nanoscale system in contact with two electrodes at different electrochemical potentials. The method is based on non equilibrium Green's functions (NEGF), that are constructed using the density functional theory Hamiltonian obtained from a given electron density. A new density is computed using the NEGF formalism, which closes the DFT-NEGF self consistent cycle.

(d) SPRKKR code

SPRKKR stands for Spin Polarized Relativistic Korringa-Kohn-Rostoker method. This code uses Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method in atomic sphere approximation (ASA) [117] which can be efficiently used to model random alloys. The idea of the CPA is to replace the random array of real on-site potentials by an ordered array of effective potentials. The scattering properties of the effective potential are then determined self-consistently in terms of the local mean-field theory with the condition that the total Green's function of the effective system does not change on replacement of the single effective potential with the real one. Many properties of disordered system can be calculated by using this code. For example electronic density of states, band structure, Fermi surfaces, magnetic exchange parameters, Auger electron spectroscopy (AES), x-ray absorption spectroscopy (XAS) etc.

4. Plan of the work

Key motivation

As we have discussed above phenomenon of superconductivity holds in it the key to many striking applications and fundamental questions regarding its mechanisms. The key parameters for applications of a superconducting material are its critical temperature (T_c), current density (J_c), and magnetic field (H_c). For applications such as superconducting cables and magnets one needs high quality polycrystalline samples with optimised properties. The exotic superconductors offer considerably high value of the critical parameters along with their interesting electronic properties.

As stated earlier cuprate materials have layered structure with T_c of the order of 100K. The nature of superconductivity in these materials is agreed to have unconventional *d*-wave symmetry. The recent discovery of superconductivity in Fe based materials has posed many important questions regarding nature of superconductivity in these materials. Therefore a comparison of electronic properties of Fe based superconducting materials with cuprates and other superconducting material will prove to be useful. Thus study of various properties of these materials not only offers many technical applications but also intriguing physics involved behind such novel properties.

High quality polycrystalline samples of various superconducting materials shall be synthesised and studied for their normal and superconducting state properties. The different experimental characterization techniques shall be employed to characterize their normal and superconducting state properties. Along with this we shall study their electronic properties using ab-initio density functional theory (DFT) to get an insight of the mechanisms involved with observed properties. Below are some of the superconducting systems proposed to be studied which are of great current research interest.

4.1 Bismuth based cuprate superconductors (BSCCO)

In case of practical applications of the superconducting materials higher values of superconducting critical parameters are desirable. The cuprates offer the highest value of superconducting transition temperature known till date [10]. Though, due to grain boundaries acting as weak links between the superconducting grains, their superconducting performance is considerably reduced [123]. Moreover, the oxygen stoichiometry in Cuprates is also a crucial parameter for determination of superconducting properties [124][125][126]. Thus it is fundamentally important to study and optimise the effect of weak links and oxygen stoichiometry in these materials.

Among various cuprate superconductors, bismuth based cuprates with general formula $Bi_2Sr_2Ca_nCu_{n+1}O_{2n+6\pm\delta}$ (BSCCO) is an important class of high temperature superconductors (HTSCs). Depending upon the value of *n*, related to number of Cu-O planes in unit cell, there can be three different stable phases of these superconductors. $Bi_2Sr_2Ca_0Cu_1O_{6\pm\delta}$ (n=0) also called Bi-2201 and having T_c ~20K, $Bi_2Sr_2Ca_1Cu_2O_{8\pm\delta}$ (n=1) known as Bi-2212 having T_c ~90K and $Bi_2Sr_2Ca_2Cu_3O_{10\pm\delta}$ called Bi-2223 with T_c ~110K. Among these materials Bi-2212 and Bi-2223 are being speculated as most promising candidates for superconducting wires and tapes that can operate above liquid nitrogen temperature. Moreover, their grains can be aligned easily either by melt processing or by mechanical deformation. However, the oxygen content affects superconducting transition temperature and normal state conductivity of Bi-2212 significantly.

Thus we plan to synthesize and study Bi-2212 with varying oxygen content and investigate in details its effect on various normal state and superconducting properties. The technique of melt quenching offers a good means to improve inter-grain connectivity resulting from reduced porosity and may also result in crystallographic alignment of grains [125][127][128]. Thus we shall also study in details how the melt quenching affects the morphology and superconducting properties of same samples. Also doping at Bi site by Pb in Bi-2212 is known to enhance superconducting performance of the single crystals, whereas on the other hand degrade it in polycrystalline samples. The cause for decreased superconducting performance of polycrystalline samples is found to be due to degraded micro texture with increasing Pb content. Thus we shall try to optimise the superconducting properties of Pb doped Bi-2212 by doping Pb at Bi site in small amounts without affecting micro texture of the samples. Bi-2223 samples will also be synthesised and their performance will be compared with optimized Bi-2212 samples. Bi-2201 shall also be synthesised and studied.

We shall also study the electronic density of states and band structure of these BSCCO superconductors by using density functional theory. The DFT studies will also be performed to study large changes in normal state properties of Bi-2212 with small variation in oxygen content. Electronic properties of Bi-2201 shall also be studied.

4.2 Some interesting conventional superconductors

MgB_2 is a superconductor with T_c of ~39K which BCS theory fails to explain within single gap scenario. The most interesting feature of MgB_2 is that it is the first material measured that exhibits two superconducting gaps [40]. Its structural analogue AlB_2 does not superconduct up to lowest measured values of temperature [129]. The multiple superconducting gaps can be measured experimentally by electronic specific heat [40] and scanning tunneling spectroscopy experiments [130]. Figure 8 illustrate both measurements for MgB_2 superconductor. Thus we shall study both the systems in details and investigate the main difference between their microscopic properties that makes them so different despite their analogous structure.

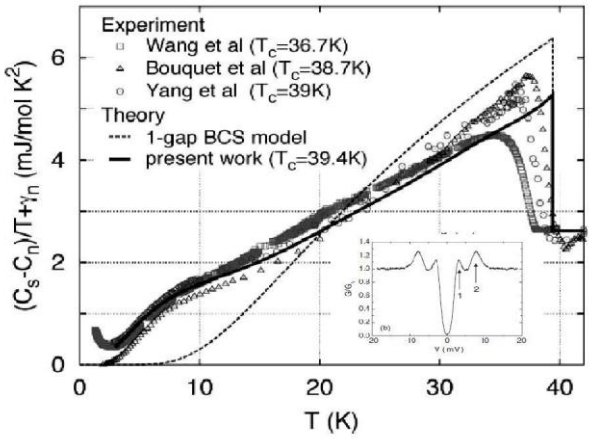

Figure 8: Illustration of two gap superconductivity in MgB_2 in electronic specific heat [40]. Inset shows same measured using scanning tunneling spectroscopy [130].

$MgCNi_3$ [131] is another interesting superconductor that has large content of Ni in its unit cell though no ferromagnetism is exhibited by it in normal state, this system is known to have ferromagnetic spin fluctuations. It has superconducting transition around 8K which is really interesting as any material close to ferromagnetism should not superconduct according to BCS. We shall study this superconductor and investigate its magnetic nature using DFT calculations.

Though Bi_3Ni is known to be superconducting below ~4.1K and studied by only few groups. A recent report by Martinez et al. [132] shows that this material is close to ferromagnetism and magnetism seems to play a role in its pairing. Though, earlier reports have shown it to be an electron-phonon type superconductor. Thus we shall revisit this material experimentally by synthesizing and looking for magnetic and superconducting properties. Moreover, we shall investigate the same theoretically using DFT for possibility of ferromagnetic ordering.

4.3 Iron chalcogenides

Among various Fe based superconductors, iron chalcogenides ($Fe_{1+\delta}Te_xSe_{1-x}$) are simplest in structure and thus offer a convenient way to study nature of superconductivity in exotic superconducting materials. Among unconventional superconductors the pairing of electrons is somehow mediated by magnetic interactions. At room temperature iron chalcogenides crystallize in tetragonal structure [133] with spacegroup *P4/nmm* (Spacegroup no. 129). Fe is located at 2a site (0.75, 0.25, 0.00) and Se/Te at 2c site (0.25, 0.25, *z*). The value of chalcogen height plays very crucial role on magnetic and electronic properties of these materials. We shall study in details the role of chalcogen species and their height above Fe layers on the magnetic and electronic properties. Moreover the role of iron at interstitial site (value of δ) plays crucial role on the magnetism of Fe layers. We shall also study the effect of interstitial iron on magnetic and electronic properties. Some of the experimental studies report ferromagnetism in thin films of FeSe the mechanism of which is still not clear as bulk FeSe does not exhibit any ferromagnetism. The possible reasons behind the ferromagnetism of these films is speculated to be because of disorder in Fe or Se planes or may be due to excess interstitial iron. We shall study the detailed nature of disorder and possibility of ferromagnetism due to disorder in these systems.

5. Work done so far

Till date we have synthesized different phases of Bismuth based superconductor viz. Bi-2201, Bi-2212 and Bi-2223. The samples have been characterized for their structural, electronic and magnetic properties. The effect of oxygen stoichiometry has been studied in details for Bi-2212 sample and superconducting properties are found quite sensitive to the oxygen content in the unit cell. We have also studied the effect of melt quenching on superconducting performance and micro-structural properties of polycrystalline samples of Bi-2212 and compared these with Bi-2223. It is found that melt quenching enhance the superconducting performance of Bi-2212 superconductor significantly.

MgB_2 is an interesting superconductor in terms of being a two gap superconductor. We have studied this superconductor using electronic specific heat and ab-initio density functional theory. We have also compared it with isostructural AlB_2 which is non superconducting. It is found that majority states at Fermi level corresponds to B-$2p_{xy}$ bands which play key role in strong electron-phonon coupling for MgB_2. The absence of these bands in case of AlB_2 shows weaker coupling of electrons via phonons and thus supports its non superconducting behaviour. $MgCNi_3$ and Bi_3Ni are speculated as ferromagnetic superconductors due to presence of Ni in them. We have studied these superconductors in details for possibility of ferromagnetism. Fixed spin moment (FSM) DFT calculations are done to find energy dependence on magnetic moment of Ni. By fitting Ginzburg-Landau equation for total energy versus magnetic moment, we have found that they are not ferromagnetic and Ni does not have any moment and thus nonmagnetic in these compounds.

The recently discovered superconducting iron chalcogenides of formula $FeTe_xSe_{1-x}$ (x=0, 0.25, 0.50, 0.75 and 1) has been studied using density functional theory. Our results show that for FeSe, LDA seems better approximation in terms of magnitude of magnetic energy whereas GGA overestimates it largely. On the other hand for FeTe, GGA is better approximation that gives experimentally observed magnetic state. It has been shown that the height of chalcogen atoms above Fe layers has significant effect on band structure, electronic density of states (DOS) at Fermi level $N(E_F)$ and Fermi surfaces.

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List of Publications:

1. "*Chalcogen height dependence of magnetism and Fermiology in $FeTe_xSe_{1-x}$*", **Jagdish Kumar**, S. Auluck, P. K. Ahluwalia and V. P. S. Awana, accepted in Superconductivity Science and Technology (2012)
2. "*Superconductivity in the vicinity of ferromagnetism in oxygen free perovskite $MgCNi_3$: An experimental and density functional theory study*" Anuj Kumar, Rajveer Jha, Shiva Kumar Singh, **Jagdish Kumar**, P. K. Ahluwalia, R. P. Tandon, and V. P. S. Awana, Journal of Applied Physics **111** 033907 (2012)
3. *"Physical property and electronic structure characterization of bulk superconducting Bi_3Ni"* **Jagdish Kumar**, Anuj Kumar, Arpita Vajpayee, Bhasker Gahtori, Devina Sharma, P. K. Ahluwalia, S. Auluck and V. P. S. Awana, Supercond. Sci. Technol. **24** 085002 (2011)
4. *"Comparative experimental and Density Functional Theory (DFT) study of the physical properties of MgB_2 and AlB_2"* Devina Sharma, **Jagdish Kumar**, Arpita Vajpayee, Ranjan Kumar, P. K. Ahluwalia, V. P. S. Awana, Letter J. Supercond. Nov Magn **24** 1925 (2011)
5. "*Anomalous heat capacity and X-ray photoelectron spectroscopy of Superconducting $FeSe_{1/2}Te_{1/2}$*" V. P. S. Awana, Govind, Anand Pal, Bhasker Gahtori, S. D.Kaushik, A. Vajpayee, **Jagdish Kumar** and H. Kishan J. Appl. Phys. **109** 07E122 (2011)
6. *"Significant Improvement in Superconductivity by Substituting Pb at Bi-site in $B_{i2-x}P_{bx}S_{r2}CaC_{u2O8}$ with x=0.0 to 0.40",* **Jagdish Kumar**, P. K. Ahluwalia, H. Kishan and V. P. S. Awana, J Supercond Nov Magn **23** 493 (2010)
7. *"Negative thermoelectric power of over-doped $Bi_2S_{r2}CaC_{u2O8}$ superconductor"* **Jagdish Kumar**, Monika Mudge[1] , G.S. Okram, Ajay Soni, V.P.S. Awana, P.K. Ahluwalia, R.B. Saxen and H. Kishan, Physica C **470** S203 (2010)

8. "*Anomalous thermoelectric power of overdoped $Bi_2Sr_2CaCu_2O_8$ superconductor*", V. P. S Awana, **Jagdish Kumar,** G. S. Okram, Ajay Soni, P. K. Ahluwalia, H. Kishan, J. Appl. Phys. **106** 096102 (2009)

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1. "*Ab-initio study of magnetism in FeSe and FeTe*" **Jagdish Kumar**, PK Ahluwalia, S Auluck and VPS Awana, DAE Solid State Physics Symposium-2011 (DAE-SSPS-2011), SRM University, Chennai, India (Dec. 2011)
2. "*Density Functional Study of Perovskite Superconductor $MgCNi_3$*" **Jagdish Kumar,** Devina Sharma, Ranjan Kumar, V.P.S. Awana and P.K. Ahluwalia International Conference on Advances in Condensed and Nano materials (ICACNM-2011), Panjab University, Chandigarh, India (Feb. 2011)
3. *"Role of inter and intra-grain connectivity on physical properties of Bi-2212 and Bi-2223"* **Jagdish Kumar**, P. K. Ahluwalia, Anurag Gupta and V. P. S. Awana International Conference On Quantum Effects in Solids of Today (I-ConQuEST-2010), National Physical Laboratory, New Delhi, India (Dec. 2010)
4. *"Difference in the microscopic properties of MgB2 and AlB2: A DFT study"* **Jagdish Kumar**, P. K. Ahluwalia, H Kishan, V. P. S. Awana ans Sushil Auluck, International Conference On Quantum Effects in Solids of Today (I-ConQuEST), National Physical Laboratory, New Delhi, India (Dec. 2010)
5. *"Composition and temperature dependence of phase stability of Bi-2201"*, **Jagdish Kumar,** VPS Awana, PK Ahluwalia, International Conference on Advanced Functional Materials (ICAFM-2009) Trivandrum, Kerla, India (Dec. 2009)

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